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Smoothed profile-lattice Boltzmann method for non-penetration and wetting boundary conditions in two and three dimensions

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ABSTRACT

In this study, the smoothed profile-lattice Boltzmann method (SP-LBM) is proposed to determine the contact line dynamics on a hydrophobic or a hydrophilic curved wall. Two types of smoothed indicator functions are introduced, namely a function that identifies the solid domain for non-slip and non-penetration conditions and a function that denotes the boundary layer for no mass-flux and the wetting boundary conditions. In order to prevent fluid penetration into the solid boundary, the fluid-solid interaction force is computed based on the definition of the fluid velocity as proposed by Guo et al. [1]. In order to implement the Neumann boundary conditions for the order parameter and the chemical potential, the fluxes from the solid surfaces are distributed to relevant physical valuables through a smoothed profile. Several two-dimensional and three-dimensional numerical investigations including those determining the Couette flows, flow around a circular cylinder, transition layer on a wetting boundary, and dynamic behavior of a droplet on a flat or curved plate demonstrate the efficiency of the present method in calculating the contact angle of a droplet on curved surfaces with wall impermeability. The present model provides a simple algorithm to compute the surface normal vector and contact line dynamics on an arbitrarily shaped boundary by using a smoothed-profile.

1. Introduction

Hydrophobic surfaces have attracted considerable attention because of significant scientific applications such as water repellency, lubricity, and self-cleaning and antifouling properties. Wettability of solid surfaces is governed by the chemical composition and the geometric structure of a surface. For example, the super-hydrophobicity of lotus leaves principally results from the presence of binary structures at both micrometer and nanometer scales and the low energy wax-like materials on the surfaces [2].

A previous study developed a phase-field model that couples Cahn–Hilliard and Navier–Stokes equations, and a good agreement was observed between the numerical results and the experimental data with respect to the spreading of a liquid droplet on a smoothed and chemically homogeneous surface [3,4]. Physical properties continuously vary in the interface between two phases in a phase-field model based on free-energy theory [5]. With respect to the study of the contact-line movement, the phase-field model sets the wetting potential that corresponds to a contact angle on the boundary, and satisfies the following three boundary conditions, namely non-slip condition, non-penetration condition, and no mass-flux condition, $\partial \mu_\phi / \partial n = 0$. Specifically, μ_ϕ denotes the chemical potential, and $\partial / \partial n$ denotes the normal derivative.

The lattice Boltzmann method (LBM) computes fluid dynamics by the evolution of distribution functions on the discrete lattice [6]. The LBM satisfies mass and momentum conservations and is suitable for computing multi-phase and multi-component flows. A color-field model and an inter-particle-potential model were proposed to easily capture irregular topological changes, interface disintegration, and coalescence in a multi-phase flow [7,8]. These models were useful in simulating contact-line dynamics by controlling the concentration on a wall [9–11]. The phase-filed model in combination with LBM was extended to consider the contact angle of a liquid placed on a flat surface by using the relation between the normal derivative of the order parameter and the wetting potential [12–14]. The difficulty in treating large density difference in the lattice Boltzmann scheme was solved such that the spreading phenomena of a droplet on a flat hydrophobic surface could be computed quantitatively [15–19]. The LBMs succeeded in verifying the effect of roughness on the wettability of a wall through the numerical simulation of droplet dynamics on a square pillar microstructure [20–22]. A bounce back on the node or half-way bounce back schemes are used in the fore-mentioned studies,

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and thus, a smooth curved boundary was approximated by a series of staircases.

Filippova proposed an interpolation method to compute the fluid flow around an arbitrarily shaped boundary in a uniform regular Cartesian mesh in the LBM [23]. This was followed by studies that enhanced the accuracy and mass conservation by the modifications of the interpolation approach of the distribution functions between a boundary and fluid nodes [24,25]. In order to obtain the distribution function reflected from a curved wall, it is necessary to compute the distance between the wall surface and the reference nodes along each discrete velocity direction in an interpolation approach. Immersed boundary-lattice Boltzmann methods (IB-LBM) can deal with an arbitrarily complex geometry by imposing a fluid-solid interaction force on Lagrangian points [26–28]. When compared to the sharp interface scheme, the IB-LBM with a diffuse-boundary approach simply obtains the fluid-solid interaction by employing a discrete delta-function to transfer quantities between the Eulerian and Lagrangian nodes [29,30]. Feng and Michaelides proposed IB-LBM based on the direct forcing method to obtain the force based on the difference between the fluid velocity and the desired velocity at the boundary without requiring a user-defined stiffness parameter [27]. Although the aforementioned explicit IB-LBMs succeeded in simulating the sedimentation of particles in an enclosure, they led to a spurious fluid mass exchange between the interior and exterior of a solid domain due to the inexactness of the non-slip boundary conditions [26–28]. Wu proposed an implicit velocity correction-based IB-LBM to provide force density and velocity correction by solving a system of equations using an inverse of matrix [31]. The IB-LBMs were proposed to accurately satisfy non-slip boundary conditions through an iterative correction of body force on the Lagrangian and Eulerian nodes [32–34]. The non-slip boundary condition was accurately enforced, and therefore, the implicit correction method succeeded in preventing the penetration of a fluid into a solid surface observed in the conventional IB-LBMs and contributed to reducing the velocity slip [35]. Most existing IB-LBMs focused on Dirichlet boundary conditions.

In order to investigate hydrodynamics on the complicated binary structured surface, Shao developed an immersed boundary-phase field-lattice Boltzmann method that embodied Neumann boundary conditions [36]. The primary concept of Shao's method involved interpreting the Neumann boundary conditions as a contribution of flux from the surface to the relevant physical variables in a control volume. The main feature of Shao's approach corresponded to the IBM that corrected the temperature on the Lagrangian points to implement Neumann (heat flux) conditions [37]. Information on the normal direction on a solid surface is necessary to examine the wettability of a solid boundary, and thus, it is necessary to compute normal directions on the Lagrangian points from the positions of the neighboring points. In the IB-LBM, it is necessary to equidistantly locate the Lagrangian points on the solid surface to form the even distribution of a solid-fluid interaction force. An adequate mesh generator and an algorithm are necessary to calculate the normal vector to the surface to simulate contact line dynamics with a lotus-leaf-like complicated geometry by the IB-LBM. With respect to the two-way coupling of an incompressible fluid with rigid bodies of an arbitrary shape, a different approach based on the smoothed-profile method (SPM) was introduced into the LBM field [38,39]. The SPM defines a spatial indicator field to yield the boundary force in Navier–Stokes equations without the Lagrangian points and without the boundary-fitted coordinate system. The indicator profile smoothly transitions between the fluid and solid regions and is a function of the distance from the solid surface [40]. It is expected that the SP-LBM can compute the normal vector to the surface from the Laplacian of the indicator profile in a manner similar to the level set method [41]. In the present study, the SP-LBM is developed to investigate the effect of surface wettability on droplet dynamics under the Dirichlet boundary conditions for velocity and under the Neumann boundary conditions for a chemical potential and for an order parameter (the phase field).

The remainder of the paper is organized as follows. Section 2 describes the SP-LBMs for incompressible single-phase and two-phase flows in detail. The section includes the techniques for reducing fluid penetration and implementing Neumann boundary conditions in SP-LBMs in two subsections. The simulation procedures are summarized. Section 3 provides numerical experiments to demonstrate the accuracy and utility of the proposed method. The cylindrical Couette flow, the fluid flow around a circular cylinder, and the axial Couette flow are calculated to validate the non-slip and non-penetration boundary conditions in two and three dimensions. In order to validate the no mass-flux and the wetting boundary conditions, we compute a transition layer on a cylinder and on a sphere, derive the equilibrium state of the contact angle of a droplet on a flat or curved plate, and predict the contact-line motion along a curved surface. Finally, concluding remarks are presented in Section 4.

2. Smoothed profile-lattice Boltzmann method

2.1. Non-slip and non-penetration conditions

2.1.1. Lattice Boltzmann method for single-phase flow

The lattice Boltzmann method for the incompressible Navier–Stokes equations uses the following kinetic equations for the distribution function f_α:

$$\tilde{f}_\alpha(\mathbf{x},t) = f_\alpha(\mathbf{x},t) - \frac{f_\alpha(\mathbf{x},t) - f_\alpha^{(eq)}(\mathbf{x},t)}{\tau_n} + \delta_t F_\alpha(\mathbf{x},t), \tag{1}$$

$$f_\alpha(\mathbf{x}+\mathbf{c}_\alpha\delta_t, t+\delta_t) = \tilde{f}_\alpha(\mathbf{x},t), \tag{2}$$

where $\tilde{f}_\alpha$ denotes post-collision value, δ_t denotes time step, $\mathbf{c}_\alpha$ denotes discrete velocity, and F_α denotes a forcing term. The fluid density and velocity are conventionally expressed in terms of the distribution function as follows:

$$\rho = \sum_\alpha f_\alpha, \qquad \mathbf{u} = \frac{1}{\rho}\sum_\alpha f_\alpha \mathbf{c}_\alpha. \tag{3}$$

The D2Q9 and D3Q19 models are used in the present study. The D2Q9 model defines the discrete velocities as follows:

$$\mathbf{c}_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ c(\pm1,0), c(0,\pm1) & \alpha = 1-4 \\ c(\pm1,\pm1) & \alpha = 5-8 \end{cases}, \tag{4}$$

where c denotes lattice velocity magnitude.

With respect to the D3Q19 model, the discrete velocity set can be expressed as follows:

$$\mathbf{c}_\alpha = \begin{cases} (0,0,0) & \alpha = 0 \\ c(\pm1,0,0), c(0,\pm1,0), c(0,0,\pm1) & \alpha = 1-6 \\ c(\pm1,\pm1,0), c(\pm1,0,\pm1), c(0,\pm1,\pm1) & \alpha = 7-18 \end{cases}. \tag{5}$$

The equilibrium distribution function is given as follows:

$$f_\alpha^{(eq)} = \omega_\alpha \rho\left[1 + \frac{3\mathbf{c}_\alpha\cdot\mathbf{u}}{c^2} + \frac{9(\mathbf{c}_\alpha\cdot\mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}\cdot\mathbf{u}}{2c^2}\right], \tag{6}$$

where ω_α denotes the weight coefficients. With respect to the D2Q9 model, $\omega_0 = 4/9$, $\omega_{1-4} = 1/9$, and $\omega_{5-8} = 1/36$. With respect to the D3Q19 model, $\omega_0 = 1/3$, $\omega_{1-6} = 1/18$, and $\omega_{7-18} = 1/36$. Conventionally, the forcing term is defined as follows:

$$F_\alpha = \omega_\alpha \rho \frac{3\mathbf{c}_\alpha\cdot\mathbf{G}}{c^2}, \tag{7}$$